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Experimental/computational approach to accommodation coefficients and its application to noble gases on aluminum surface

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Abstract

A technique is proposed to assess gas-surface accommodation coefficients. The technique utilizes the fact that radiometric forces exerted on heated objects immersed in rarefied gases are governed by the interaction of gas molecules with the surface. In the present implementation, it connects measurements of radiometric forces on a heated vane in the transitional flow regime with the kinetic modeling of the flow, and derives the accommodation coefficients through the successive analysis of measured and computed results. A new combined ES-BGK / DSMC approach that allows accurate and time efficient analysis of radiometric forces on a vane in large vacuum chambers filled with rarefied gas is presented. Accommodation coefficients for the Maxwell model are estimated for argon, xenon, and helium on a machined aluminum surface, and found to be 0.81, 0.86, and 0.53, respectively.

INTRODUCTION

The history of accommodation coefficients of energy and momentum of gas molecules colliding with solid surfaces spans well over a century [1]. Its beginning dates to the work of Kundt and Warburg [2] who studied the effect of gas density change on the damping of a vibrating disk. The viscosity appeared to decrease with density, which seemed unexplainable at the time. The authors suggested an incomplete interaction, or accommodation, of gas molecules at the surface, where a low density gas slips over a surface. Following that work, Maxwell showed [3] that the slip phenomenon has roots in kinetic theory, and he treated the solid wall as something intermediate between a perfectly reflecting and a perfectly absorbing surface. He proposed that "of every unit of area a portion α absorbs all the incident molecules, and afterwards allows them to evaporate with velocities corresponding to those in still gas at the temperature of the solid, while a portion $1-\alpha$ perfectly reflects all the molecules incident upon it" [3].

The model proposed by Maxwell is in fact the first theoretical model that describes gas-surface interaction, and it is still widely used today both in experiment and numerical simulation. According to the Maxwell model, the velocity distribution function of reflected molecules may be written as a function of the accommodation coefficient α (see, for example, [4])

$$f_r(t,\mathbf{x},\mathbf{v}_r) = (1-\alpha) f_i(t,\mathbf{x},\mathbf{v}_r - 2(\mathbf{v}_r\cdot\mathbf{n})\mathbf{n}) + \alpha\left(\frac{\beta_r^2}{\pi}\right)^{3/2} \mathrm{e}^{-\beta^2\mathbf{v}_i^2}, \tag{1}$$

where f is the distribution function, t is time, $\mathbf{x}$ and $\mathbf{v}$ are molecular position and velocity vectors, respectively, and $\mathbf{n}$ denotes the surface normal. Subscripts i and r refer to incident and reflected molecules, respectively, and $\beta = \sqrt{\frac{m}{2kT_r}}$. The first term in Equ. (1) refers to specular reflection, and the second term refers to diffuse reflection. The reflected temperature, T_r, is the wall temperature, T_w, according to the original Maxwell's idea, but may generally be a free parameter of the model.

The tangential momentum transferred to the surface by the incident molecules may be written [4]

$$\mathbf{P}_{i\tau} = -m \int\limits_{\mathbf{v}\cdot\mathbf{n}<0} f_i \mathbf{v}_{i\tau}(\mathbf{v}_i\cdot\mathbf{n})\mathrm{d}\mathbf{v}_i, \tag{2}$$

where the subscript τ refers to the tangential to the surface components of molecular velocity,

and the tangential momentum of reflected molecules is then

$$\mathbf{P}_{r\tau} = -m \int\limits_{\mathbf{v}\cdot\mathbf{n}>0} f_r \mathbf{v}_{r\tau}(\mathbf{v}_r \cdot \mathbf{n}) d\mathbf{v}_r = (1-\alpha)\mathbf{P}_{i\tau}. \tag{3}$$

These equations show that the accommodation coefficient used in Eqn. (1) may be considered as the coefficient of accommodation of the tangential momentum, and may be written as

$$\alpha \equiv \alpha_\tau = \frac{P_{i\tau} - P_{r\tau}}{P_{i\tau}}. \tag{4}$$

The accommodation coefficients for the normal momentum and energy may be introduced similar to Eqn. (4) as

$$\alpha_n = \frac{P_{in} - P_{rn}}{P_{in} - P_w}, \quad \alpha_E = \frac{E_{in} - E_{rn}}{E_{in} - E_w}, \tag{5}$$

where the subscript w refers to the surface properties, or the properties that would have had a gas at equilibrium with the wall.

Although the Maxwell model is still the most widely used model of gas-surface interaction, other models have also been proposed. Here we mention only a two-parameter Cercignani-Lampis model [5] that uses two accommodation coefficients, α_τ and α_n, and a multi-parametric Nocilla model [6] in which the velocity of reflected molecules is simulated by the function

$$f = n_r \pi^{-3/2} c_r^{-3} \exp\left\{-c_r^{-2}\left[\vec{\xi} - c_r \vec{S}_r\right]^2\right\}, \quad c_c = \sqrt{2\,k/m\,T_r}, \quad \vec{S}_r = \vec{\xi}/c_r.$$

The four parameters $\vec{S}_r \equiv (S_{nr}, S_{\tau r})$, T_r, n_r of this function are determined from experimental data.

The development and utilization of different gas-surface interaction models is related to various application areas where such interactions are important. One area of interest is the high altitude aerodynamics, and, in particular, free-molecular aerodynamics of satellites (see for example, [7]). For the latter application, the Nocilla model is often used. The importance of the gas-surface interaction model in this case is obvious, since the collisions of molecules with the spacecraft surface are the dominant process that influences drag, lift, and heat loads.

Another area where the gas-surface processes are important is gas flows in micro and nanoscale devices. In such devices, the gas mean free path is comparable to characteristic flow dimensions, and the consideration of kinetic effects is essential for accurate prediction of

device performance and peculiarities. The large surface-to-volume ratio further increases the influence of the wall. Note that for microscale flows, the preservation of the detailed balance in collisions of gas molecules with solid interfaces is critical. Therefore, the Nocilla model, which does not satisfy this requirement, is not a good choice, and the Maxwell or Cercignani-Lampis models are better suited for the description of low speed flows in microdevices. Beside these two areas, gas-surface interaction is important, if not determining, in many other applications. Near-continuum supersonic flows over sharp leading edges, contamination problems, and two-phase flows [8] are just a few examples of such applications.

Accurate prediction of the above flows requires the researcher not only to select an appropriate gas-surface interaction model, but also to specify the parameters of this model for each type of gas species - solid wall interface. Two principal approaches are used to determine parameters of the model, theoretical and experimental. The theoretical approach is usually based on the detailed studies of molecular interactions using classical or quasi-classical trajectory calculations in the framework of the molecular dynamics method [9]. In the experimental approach, parameters of the selected interaction model are estimated directly from the measurement. The parameters for the Nocilla model, for example, are usually obtained from molecular beam experiments or flight experiments (see, for example, [10], [11], and references therein). In Ref. [12], a connection between the exit velocity distribution given by the Nocilla model, and the classical momentum and energy accommodation coefficients were given.

The advantage of the molecular beam technique is that it may provide detailed information on the velocity distributions of reflected molecules. There are many situations, however, when such detailed information is not necessary, and the knowledge of accommodation coefficients, either momentum or energy, would suffice. Examples include the force estimate of spacecraft at high altitudes, or the evaluation of heat loads in microdevices. Over the last three decades, molecular beam experiments have been used extensively to determine both the normal and tangential momentum and energy accommodation coefficients [13][14],[15] for various gas-surface pairs. For the energy (thermal) accommodation coefficient, parallel plates, co-axial cylinders, and hot-wire methods have been widely used. A comprehensive review of different approaches to the thermal accommodation coefficient measurements may be found in Ref. [16]. Among many papers where thermal accommodation was studied, only the recent work in Ref. [17] will be mentioned here. In Ref. [17], the accommodation

of helium, nitrogen, and argon was studied on several differently treated engineering surfaces. Various experimental techniques used in the past to measure tangential momentum accommodation coefficient, such as the rotating cylinder method, the spinning rotor gage method, the flow through microchannel approach, as well as the molecular beam technique, are discussed in recent review article [18].

As compared to high-enthalpy flows around space vehicles, gas-driven flows in microscale devices are characterized by relatively low gradients in gas velocity and temperature, and the velocity distribution function in these flows is often close to Maxwellian. As a result, prediction of gas-driven flows in such devices typically requires knowledge of momentum and/or energy accommodation coefficients as a function of gas and surface temperature. The use of molecular beam technique may be quite difficult in this case, since the after-collision velocities need to be analyzed for a large number of pre-collisional energies. On the other hand, standard techniques for the accommodation measurement may not be applicable when information on momentum accommodation, normal or tangential, is needed.

One major issue with the need of gas-surface interaction parameters to predict complicated flow interactions is the range of experimental data for similar flows. For example, various experiments can have different, and in some cases conflicting, results. Take, for instance, the measurement of the energy accommodation of helium on a platinum surface. Results in Refs. [20], [21], and [22] can vary by more than 30%. Although these results are rather historical, it highlights the current need to re-investigate these data sets in order to study the effects of gas temperature, surface temperature, surface preparation, gas adsorption on surfaces, and gas pressure.

The objective of this work is to evaluate the feasibility of using a new technique for measurements of momentum accommodation coefficients, based on the combined experimental and computational analysis of radiometric forces on heated plates. Radiometric forces are typically exerted on nonuniformly heated objects immersed in rarefied gases, and tend to move these objects in the direction from the cold to the hot side. The authors of Ref. [19] have recently remarked that the measurement of radiometric forces may yield data on gas-surface interaction. However, there are two problems that make the direct use of such measurements to infer momentum accommodation coefficients extremely difficult. First, there are usually molecular collisions present in radiometric flows, and these collisions do not allow simple and accurate analytic evaluation of accommodation coefficients from force

measurements beyond the free molecular regime. Second, while the availability of force measurements in free molecular regime would offer the benefit of accommodation coefficient evaluation, there is a physical limitation in the accuracy of such measurements. The fewer gas-surface collisions a radiometer vane experiences, the greater the experimental error. To avoid these difficulties, it is suggested in the present work to measure radiometric forces in the transitional regime, and then use kinetic modeling of radiometric flows to infer the momentum accommodation coefficients.

RADIOMETRIC APPROACH TO MOMENTUM ACCOMMODATION STUDY

The radiometric forces on a heated plate may be described analytically only in a free molecular regime; the presence of even relatively small number of molecular collisions in the transition regime complicates the flow to the point where accurate analytical description is not possible, and a numerical approach has to be used to address the problem. Even for a free molecule flow, some model needs to be used for the gas-surface accommodation in order to make analytical treatment possible.

Generally, for a plate with its opposite sides heated uniformly to different temperatures T_h and T_c, the forces in the direction normal to the plate, created by molecules reflected from the hot and the cold sides of the plate, may be written

$$F_h = n_h m \int_{\mathbf{v}\cdot\mathbf{n}} f_h \mathbf{v}_{rr}(\mathbf{v}_r \cdot \mathbf{n}) \mathrm{d}\mathbf{v}_r \quad \text{and} \quad F_c = n_c m \int_{\mathbf{v}\cdot\mathbf{n}} f_c \mathbf{v}_{rr}(\mathbf{v}_r \cdot \mathbf{n}) \mathrm{d}\mathbf{v}_r, \tag{6}$$

where subscripts h and c refer to the hot and cold sides, respectively. The number density that describes the flux of reflected molecules may be obtained from the assumption of the equality of the incident and reflected mass flux (i.e. no sticking on the surface),

$$n_{h,c} \int_{\mathbf{v}\cdot\mathbf{n}} f_{h,c}(\mathbf{v}_r \cdot \mathbf{n}) \mathrm{d}\mathbf{v}_r = n_g \int_{\mathbf{v}\cdot\mathbf{n}} f_g(\mathbf{v}_r \cdot \mathbf{n}) \mathrm{d}\mathbf{v}_r, \tag{7}$$

where subscript g refers to the incident gas molecules. In a free molecular flow, the Maxwellian distribution function of f_g may be reasonably assumed. For fully diffuse accommodation, the number density of reflected molecules is obtained by integrating Eqn. (7) over equilibrium distribution functions to give

$$n_{h,c} = n_g \sqrt{\frac{T_g}{T_{h,c}}}, \tag{8}$$

where index h, c refers to either hot or cold side of the plate. The force on the side of the plate will be

$$F_{h,c} = \frac{p_g}{2} + \frac{p_g}{2}\sqrt{\left(\frac{T_{h,c}}{T_g}\right)}, \tag{9}$$

where p_g is the gas pressure. The first term in Eqn. (9) is for the incident molecules, and the second term accounts for the contribution from the reflected molecules. If the accommodation coefficient is introduced according to the expression suggested by Knudsen [23]

$$\alpha_K = \frac{T_g - T_r}{T_g - T_w}, \tag{10}$$

then, assuming the same accommodation coefficient on the hot and cold sides of the plate (a small temperature difference between the plates), and using T_w from Eqn. (10) instead of T_h and T_c in Eqn. (9), one can obtain the expression for the total radiometric force on the plate

$$F_K = \frac{p_g}{2}\left(\sqrt{\frac{(1-\alpha_K)T_g + \alpha_K T_h}{T_h}} - \sqrt{\frac{(1-\alpha_K)T_g + \alpha_K T_c}{T_c}}\right). \tag{11}$$

Note that the contributions from the incident molecules cancel out in the free molecular flow; the force is directed from the hot to the cold surface.

If the Maxwell model of gas surface interaction is used, then, substituting Eqn. (1) into Eqn. (6) and making use of Eqn. (7), one can obtain for the free molecular force

$$F_M = \alpha\frac{p_g}{2}\left(\sqrt{\frac{T_h}{T_g}} - \sqrt{\frac{T_c}{T_g}}\right). \tag{12}$$

Therefore, the free molecular radiometric force calculated using the Maxwell model is linearly dependent on the tangential momentum accommodation coefficient. If the momentum accommodation coefficient in the Maxwell model, α, is close the energy accommodation coefficient in the Knudsen model, α_K, then the force predictions obtained with Eqn. (11) and Eqn. (12) are similar for small temperature differences. The difference between them becomes significant when the surface temperatures are not similar. Equation 12 allows one to easily calculate the accommodation coefficients when the radiometric force in the free molecular regime can be measured.

In reality, however, it is difficult to accurately measure the radiometric force in free molecular regime. Such measurements are possible for a transitional regime, for which the above analytic expressions are not applicable. Therefore, it is reasonable to infer the

accommodation coefficients from a numerical simulation performed for a given gas-surface interaction model with varying parameters of the model. It is clear that the conventional continuum approaches of the computational fluid dynamics, such as those based on the solution of the full Navier-Stokes equations or boundary layer equations, can not be used to compute radiometric forces in the transitional flow regime. In these approaches, developed for modeling gas flows close to equilibrium, the effects of rarefaction are typically accounted for through the boundary conditions of slip velocity and temperature jump on the surface. The assumption of small deviation from equilibrium makes them inapplicable for modeling radiometric flows and calculating radiometric forces. In this case, a kinetic approach based on the solution of the Boltzmann equation has to be used. For a kinetic approach, a kinetic model of gas surface interaction needs to be used, such as the Maxwell model, and the approach naturally gives the velocity distribution functions for the incident and reflected molecules.

Thus, in order to obtain the accommodation coefficients for a given gas-surface interaction model, numerical results need to be obtained by comparing results from a kinetic approach for a computational setup that closely reproduces the experimental one. The details on the present experimental setup are given in the following section.

EXPERIMENTAL SETUP

As radiometric phenomena occur in rarefied conditions, there are only two ways to study them experimentally. The first is to build extremely small devices on the order of nanometers and test them under atmospheric conditions. The second way is to build a larger device and modify the background pressure such that the local Knudsen number is large enough for the flow to be considered transitional (i.e. Kn > .01). In this work the latter method has been chosen, and all the experimental results that follow have been achieved under low pressure conditions in a large 3.0 m diameter vacuum chamber. The use of such a large chamber is critical to avoid the effect of chamber walls that was found to strongly impact the radiometric force in smaller chambers [25].

To accurately measure the impact of various accommodation coefficients, and to be practical to model using an axisymmetric code, a circular radiometer vane with a diameter of 11.13 cm was used. The vane consisted of a Teflon insulator sandwiched between two alu-

minum plates with a resistive heater located between one of the plates and the insulator. The temperature of one side of the device was maintained by varying the power input to the heater, while the temperature of the opposite side was not acively maintained and was allowat to float. Each of the three pieces of the radiometer vane had a thickness of 0.32cm, and when assembled yield a total device thickness of 0.96cm.

One motivation for this particular configuration of radiometer vane comes from historical work [26] where rudimentary temperature measurements of the vanes suggested that a significant temperature drop occurred at the outermost edges. This same work made it quite clear that to accurately deduce a theory for the operation of the radiometer, it would be necessary to discover exactly what effect the temperature variations at the edges had. For the sake of clarity it should be noted here that there are two gradients important to the flow: the first of these shall be referred to as the radial gradient and will refer to the temperature profile of a plate from the center to the periphery, while the second will be called the axial gradient and will to refer to temperature profile along an axis normal to the face. In an ideal experiment, the axial gradient would be large and the radial gradient would be non-existent such that the experiment and simulation share nearly identical temperature profiles. It is for these reasons that the particular aluminum "sandwich" design was chosen; not only does the high thermal conductivity maximize the surface temperature of the hot plate (and thus the axial temperature gradient), but it also minimizes the radial temperature gradients near the edges of the device.

To measure the force produced by this device, it was mounted on a modified nano-Newton Thrust Stand(nNTS)[27] located inside the vacuum chamber. A schematics of the experimental setup is shown in Fig. 1. Here, every effort was made to minimize the impact of the thrust stand arm and attachment mechanism by using 6.35 mm tubing coupled with a 2 x 40 mm threaded rod. When calibrated using a pair of electrostatic combs[28], the nNTS provides very accurate and repeatable data with typical force resolution of approximately 0.1μN and statistical scatter of about 1%. For the preliminary experiment, the experimental error based on standard deviation ranges from a few percent at the lowest pressures to less than 1% through most of the curve. However, due to the normalization by experimental temperature measurements and the small uncertainty of the calibration method, the total absolute experimental uncertainty is $\approx 4\%$. Day-to-day variation of multiple data sets has been observed to be $\approx 1\%$.

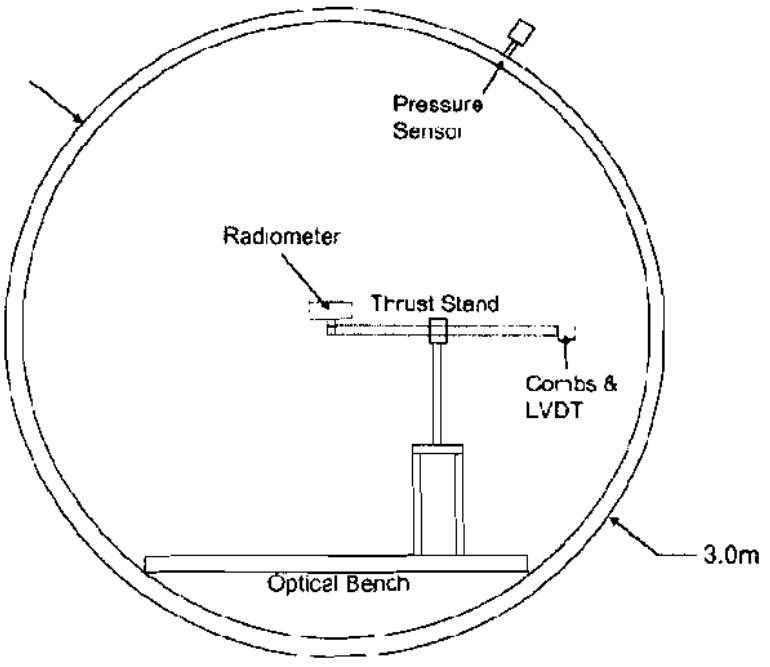

FIG. 1: Setup of the radiometric experiment.

The experimental data was obtained by evacuating the vacuum chamber to a base pressure below 10^{-3}Pa. This low pressure was required to minimize the impact of the background gas to a level low enough as to be inconsequential to the measurements being made. While the evacuation of the chamber was taking place, a constant voltage was applied to the heater. This resulted in the main radiometer surfaces reaching temperatures of approximately 419 K (hot) and 394 K (cold), though the exact values fluctuated depending on both the species and pressure of the background gas. Force measurements were made by varying the background pressure of the gas in the chamber, where argon, helium, and xenon were all used. The highest background pressure achieved was approximately 1.6 Pa, but varied depending on the molecular weight of the background gas.

NUMERICAL MODELING OF RADIOMETRIC FLOWS: A COMBINED KINETIC APPROACH

There are several challenges of modeling radiometric flows in the transitional regime, most of which are related to the low speed nature of these flows. The principal challenges are the subsonic boundary conditions, low signal-to-noise ratio, and very long time to reach

steady state. The first problem may be overcome when a closed system is considered; in this case, the wall boundary conditions may be imposed on the boundaries of the computational domain. However, the study of the accommodation coefficients implies that a very large chamber needs to be considered to avoid the impact of the chamber walls (similar to the experimental setup discussed in the previous section). The physical problem of the boundary conditions is therefore replaced by a computational problem of a large simulation domain. The low signal-to-noise ratio is mostly a challenge for statistical kinetic approaches, such as the direct simulation Monte Carlo (DSMC) method [24]. Very long times to reach steady state create difficulties primarily for time-accurate approaches where the use of an implicit method may drastically reduce this challenge.

There are a number of kinetic approaches that are generally capable of predicting radiometric flows; they all differ in the degree of precision and the computational cost. At present, the most powerful and widely used kinetic approach to the solution of the Boltzmann equation is the DSMC method. This approach however suffers from high computational cost when low-speed flows need to be modeled. The main problems associated with this method are long times to reach steady state and low signal-to-noise ratios. There is a number of alternative DSMC-based approaches proposed to deal with the problem of low signal-to-noise ratio that allow significant reduction in macroparameter sampling time compared to the standard DSMC method (see, for example, [29, 30]). Although all these techniques do allow significant reduction in the steady-state time averaging cost, they do not deal with the reduction of computational cost associated with the long time to reach steady state, which is often the main issue for modeling radiometric flows. The direct numerical integration of the Boltzmann equation [31], while avoiding the signal-to-noise ratio problem, may be impractical when millions of time steps and tens or hundreds of thousands of cells have to be modeled.

A plausible numerical alternative for such flows appear a deterministic solution of a simplified form of the Boltzmann equation known as a kinetic model equations. Bhatnagar-Gross-Krook (BGK) [32] and ellipsoidal statistical (ES) [33] kinetic models use a non-linear relaxation term instead of the full Boltzmann collision integral, and possess the same collision invariants as the Boltzmann equation. Both BGK and ES models satisfy the H-theorem expressing the increase of entropy of gas under consideration. The ES model seems preferable as it allows one to use the correct Prandtl number, whereas the Prandtl number for the BGK

model is unity. The primary advantage of this numerical alternative is its high computational efficiency.

Numerical analysis has been conducted using the DSMC and ES BGK methods in order to assess their applicability to modeling of radiometric flows in general, and the experimental setup described in the previous section, in particular. The computational tool SMILE [34] was used to obtain the solutions with the DSMC method. In DSMC runs, the variable soft sphere model (VSS) with parameters listed in Ref. [24] was used for the molecular collisions, and the Maxwell model was used to calculate gas-surface collisions. A finite volume solver SMOKE [35] has been used to deterministically solve the ES model kinetic equation. SMOKE is a parallel code based on conservative numerical schemes developed by L. Mieussens [36]. A second order spatial discretization was used. The solutions were typically obtained in two successive steps. First, an implicit time integration scheme was ran until the result is converged. Second, a conservative explicit time integration scheme was used with the initial conditions from the first step. This two-step approach allowed up to two orders of magnitude reduction in computational time compared to an explicit-only case.

The computations presented in this section were conducted in a two-dimensional chamber of 0.44m×0.44m. The size of the vane was 0.04m×0.01m. The vane temperatures were 450 K and 410 K for the hot and cold sides, respectively. A chamber wall temperature of 300 K was assumed. The use of a much smaller chamber was necessary as the DSMC computations of radiometric flows are very costly from the computational standpoint. A typical DSMC run of the small chamber took up to four days on a 40 processor parallel computer in order to achieve a below 2% statistical accuracy in the radiometric force calculations. It is clear that DSMC modeling of the entire experimental facility, with a volume that is two orders of magnitude larger than that of the small chamber, is impractical.

The computations were performed for pure argon. The results for a stagnation pressure of 0.609 Pa are presented in Fig. 2, where the translational temperature fields are presented for the ES-BGK (upper half) and DSMC (lower half) solutions. As expected, the gas temperature significantly increases near the vane. For this pressure, which corresponds to the Knudsen number of approximately 0.25 based on the vane length, the temperature jump on the surface is about 40 K for the hot side, and 30 K for the cold side. At the chamber walls, the temperature jump is about 2 K. The main conclusion from the comparison of the

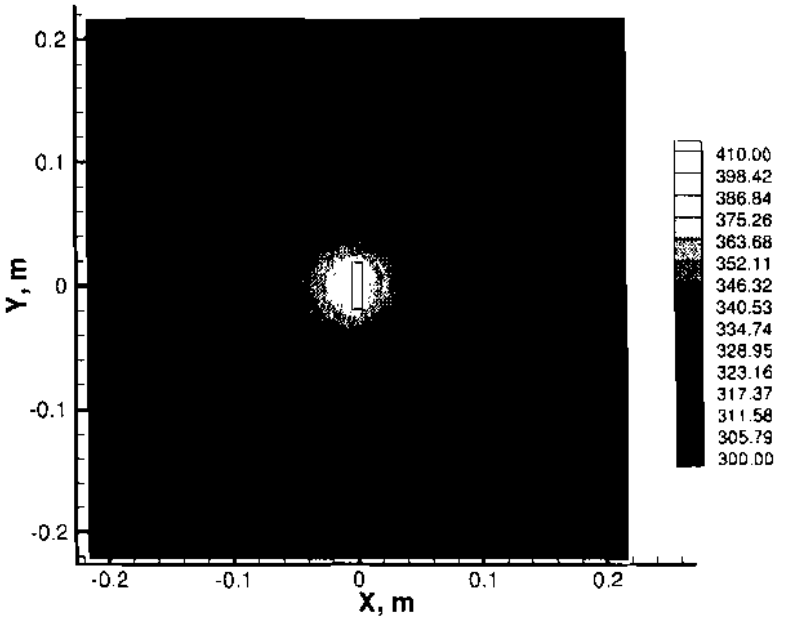

FIG. 2: ES-BGK (top) and DSMC (bottom) translational temperature fields.

two solutions is that they agree very well, both in the regions close to the vane and near the chamber walls. The difference between the solutions is less than one degree Kelvin, which is reasonably small compared to the temperature variation from chamber walls to the radiometer vane, which exceeds 100 K.

Comparison of the argon number density fields for the two approaches is given in Fig. 3. There is generally a very good quantitative agreement between the DSMC and ES-BGK solutions. The difference does not exceed a few tenths of a percent, which is within the numerical error of the calculations mostly related to the spatial and time discretization, as well as the number of molecules in the DSMC method.

Good agreement between the macroparameters obtained with the statistical and deterministic kinetic approaches allows one to assume equally good agreement between the surface properties. The pressure forces calculated are indeed very close both for the hot and the cold sides of the plate. For the DSMC calculation, the integral pressure force is 2.4928×10^{-2} N and 2.4627×10^{-2} N for the hot and the cold sides, respectively. For the ES-BGK calculation, these values are 2.4926×10^{-2} N and 2.4664×10^{-2} N. However, the radiometric force is based on the difference between the hot and the cold side forces, giving 3.01×10^{-4} N in DSMC and 2.62×10^{-2} N in ES-BGK. Therefore, the difference in the radiometric forces is almost

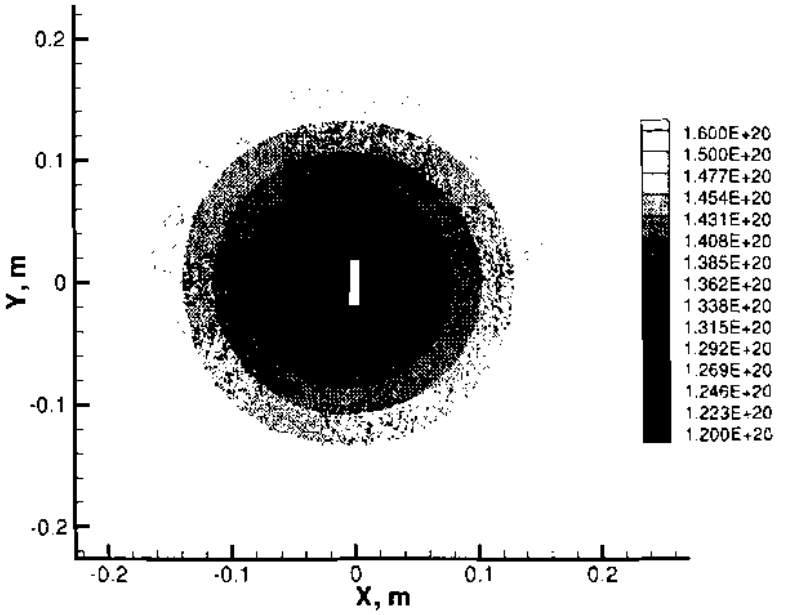

FIG. 3: ES-BGK (top) and DSMC (bottom) number density fields.

15% between the two numerical techniques. The radiometric force only amounts to about one percent of the pressure force on the hot surface, and its accurate calculation is difficult. The results for the radiometric pressure-based force on the vane are given in Fig. 4. These results show that the DSMC and ES-BGK forces coincide in the free molecular regime, as expected, and are close for larger pressures (for Knudsen numbers smaller than 0.1). However, for intermediate pressures the DSMC values are systematically higher, with the maximum difference observed at 0.609 Pa. This can be attributed the deviation of the BGK solution from DSMC by the approximations inherent in the ES-BGK model equation as compared to the full Boltzmann equation that is solved statistically with the DSMC method. The collision operator of the model kinetic equation is such that the relaxation of molecules that have different velocities occurs at the same speed; in addition, the relaxation of molecules after collisions to the local Maxwellian distribution may not be a satisfactory assumption under strongly non-equilibrium conditions.

Accurate modeling of flow macroparameters and significant overprediction of the radiometric force by the solution of the ES-BGK equation indicates that the approach may be used for a qualitative analysis of radiometric phenomena, but not for the quantitative prediction of gas-surface accommodation parameters through the comparison with experimental data. On the other hand, the use of the DSMC method to compute radiometric forces in

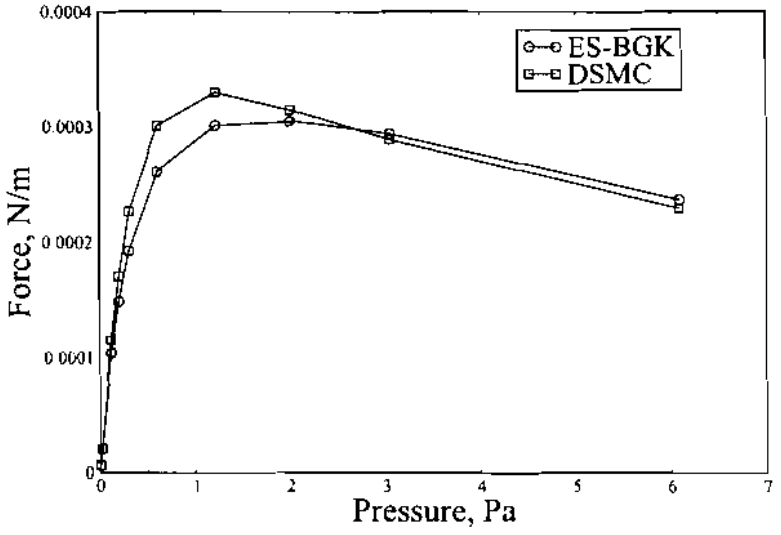

FIG. 4: Radiometric forces on the plate obtained with ES-BGK and DSMC.

large chambers, necessary to avoid chamber wall effects, is prohibitively computationally expensive. A reasonable alternative appears to be the use of a combined ES-BGK/DSMC approach, where the final solution is obtained in two successive steps. First, an ES-BGK modeling is conducted in a large computational domain that includes both the radiometer vane and the chamber walls. The solution of this first step is used to set the boundary conditions for the second step. At the second step, the DSMC method is applied in a much smaller domain, with the subsonic boundary conditions taken from the first step.

There are a number of ways to specify the boundary conditions for DSMC. The easiest one is to directly use the four macroparameters (density, temperature, and two velocities) from the ES-BGK solution in the DSMC simulations. In this case, the velocities of molecules entering the DSMC computational domain are sampled from the Maxwellian distribution with parameters from the ES-BGK solution. Another possibility is to use directional temperatures obtained from the ES-BGK solution, and sample velocities of new molecules in DSMC from the ellipsoidal distribution function. Finally, the most accurate, and the most cumbersome, way to set the DSMC boundary conditions is to use the velocity distribution functions from the solution of the model kinetic equation.

One way to examine the applicability of various approaches to the boundary conditions is to apply a combined ES-BGK/DSMC method to a test case where a reliable DSMC solution is available for the entire chamber, and then compare the obtained results. In this work,

the DSMC solution presented earlier in this section was chosen as the validation tool for the combined approach. The computational domain for the DSMC step of the combined approach was set to 0.22m×0.22m (one half of the full chamber size in each direction). The range of pressures from 0.3 Pa to 3 Pa was considered in order to examine the flow regime where the difference in radiometric force between the DSMC and ES-BGK methods is significant. For the case under consideration, analysis of nonequilibrium between the directional temperatures showed that the difference between T_x and T_y along the boundaries of the DSMC domain in the combined approach does not exceed 0.2%, and typically is less than 0.1%. Because of this, the approaches based on Maxwellian and ellipsoidal distributions of incoming molecules are expected to produce results that agree within the numerical error of the computations. Therefore, only the Maxwellian distribution was used below.

It is much more important to separate the incoming and outgoing molecules in the ES-BGK solution when setting up the boundary conditions for the second-step DSMC simulation. The gas temperature of the incoming molecules is significantly (several percent) smaller than that based on both incoming and outgoing molecules. The resulting pressure force for the combined ES-BGK/DSMC approach that uses either total incoming and outgoing molecules or the incoming molecules alone is given in Table I. The corresponding DSMC values are also shown in this table. The incoming molecule based ES-BGK/DSMC force practically coincides with the benchmark DSMC values for lower and higher pressures. It is slightly larger than the DSMC near the maximum. The force obtained using the total properties is larger for all pressures under consideration; the difference is especially significant for higher pressures. Good agreement between the incoming properties based ES-BGK/DSMC approach and the DSMC-only solution proves that the combined method may be used for the evaluation of momentum accommodation coefficients.

EVALUATION OF ACCOMMODATION COEFFICIENTS

Good agreement between the full DSMC and the combined kinetic approach presented in the previous section allows the authors to apply the combined approach to analyze radiometric flows in a large vacuum chamber. A 3 m cylindrical chamber is simulated in this work, whose geometry with good accuracy reproduces the companion experimental setup. The radiometer size and location inside the chamber, as well as the temperature conditions, also

Pressure, Pa	DSMC	ES-BGK/DSMC incoming	ES-BGK/DSMC total
0.305	2.27e-4	2.28e-4	2.33e-4
0.609	3.01e-4	3.00e-4	3.07e-4
1.219	3.30e-4	3.40e-4	3.56e-4
2.000	3.15e-4	3.26e-4	3.38e-4
3.046	2.89e-4	2.85e-4	3.32e-4

TABLE I: Comparison of radiometric forces (N) obtained with different approaches.

correspond to those used in the experiment. Diffuse reflection with a complete energy and momentum accommodation was assumed on the chamber walls and the surface of the vane (with one exception explained below). Since the experimental setup closely approximates a flow with an axial symmetry, axisymmetric ES-BGK and DSMC codes were used in these computations. The subsonic boundaries of the DSMC computational domain were located 30 cm from the vane both in the axial and radial directions. A somewhat larger domain was used as compared to the test case considered in the previous section to avoid the impact of the boundaries. Note that due to the axial symmetry of the flow, the temperature at the inflow boundaries in DSMC was only a few degrees higher than the ambient temperature of 300 K.

Three gases were considered in this work, argon, xenon, and helium. The radiometric forces for these gases, obtained with the combined ES-BGK/DSMC approach as well as measured experimentally, are presented in Fig. 5. Generally, the radiometric force consists of two components, (i) the total radiometric force that includes the force resulting from the pressure difference between the hot and the cold sides of the vane, and (ii) the shear force on the lateral (circumferential) side of the vane. To show separate contribution of these forces, two sets of numerical results are shown, the total radiometric force that includes both components, and the radiometric force that is based on pressure alone. The results show that the shear force is a minor factor for pressures smaller than 0.6 Pa for argon, where the maximum force is observed. It becomes more significant for larger pressures, for which the contribution of the lateral side of the vane can not be ignored. It may appear preferable to analyze the accommodation coefficients under conditions where the lateral side has a

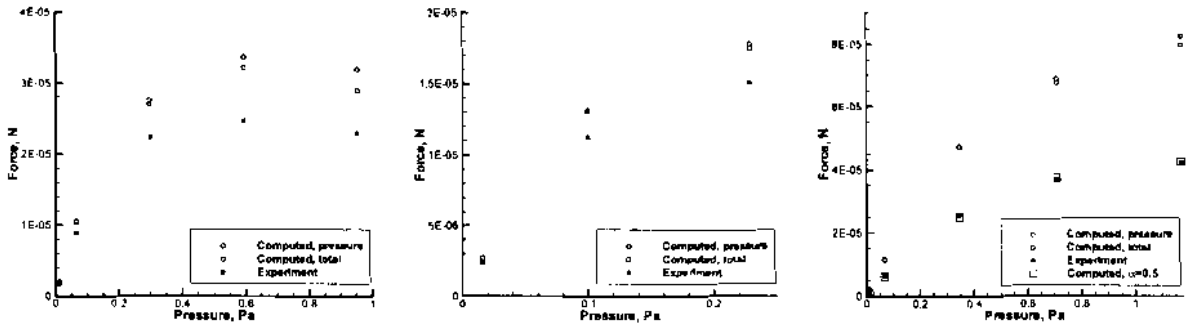

FIG. 5: Experimental and computed radiometric force for argon (left), xenon (center), and helium (fight).

negligible effect, such as a much thinner vane, but it is difficult to realize in the experiment.

For all three gases, the experimental data lay lower than the numerical points, which is a clear indication of an incomplete surface accommodation. Beyond that, several other factors may play a role in this difference. First, there are numerical and experimental errors; they are not expected to cause a difference between the computation and the measurement larger than 5%. Then, there is a finite chamber size, with unknown accommodation on chamber walls. This has been found to be a minor issue in a series of ES-BGK calculations, where the chamber size larger than about 2m was found to have a negligible effect on the radiometric force. Finally, there is some impact of intermolecular collision law, or, in other words, gas viscosity and heat conductivity. This factor is also believed to be minor, as the bulk gas properties correspond to well established experimental values for the temperature range under consideration. All this indicates that the gas accommodation on the vane surface is the main reason for the difference between the numerical and experimental values. For comparison, additional computations were conducted for helium, where the difference between the modeling and the data is greatest, using the Maxwell model with an accommodation coefficient of 0.5. It is clearly seen that the use of a lower accommodation coefficient allows one to obtain good agreement with experimental data for all pressures considered.

The value of 0.5 for accommodation coefficient used for helium to reproduce the experimental data is in fact close to the experimental-to-computed ratio of 0.53 obtained after averaging over pressures. Remember that the Maxwell model is characterized by a linear dependence between the force and the accommodation coefficient; obviously, the dependence

is close to linear in the transitional regime as well. The value of 0.5 may in fact be obtained if the Knudsen model of accommodation is assumed, and the functional dependence of Eqn. 11 is applied. In this case, the unknown α is calculated by equating the ratio of the right hand sides of Eqn. 11 with $\alpha_K = \alpha$ and $\alpha_K = 1$ to the experimental-to-computed force ratio. Note that the value 0.5 is obtained when the Knudsen model of accommodation is assumed, and the functional dependence of Eqn. 11 and equating the ratio of the right hand sides of Eqn. 11 with an unknown α_K and $\alpha_K = 1$ to the experimental-to-computed force ratio.

Interestingly, the value of 0.5 also coincides with that of the Knudsen model of accommodation obtained assuming the functional dependence of Eqn. 11 and equating the ratio of the right hand sides of Eqn. 11 with an unknown α_K and $\alpha_K = 1$ to the experimental-to-computed force ratio. As was mentioned earlier, the difference between the accommodation coefficients defined by the Maxwell model and the Knudsen expression is small for relatively small temperature differences examined in this work. It is therefore impossible to state which one is a better approximation for the transitional regime. For kinetic approaches, the authors believe that the use of Eqn. 12 may be a better fit, with a simple ratio between the experimental and numerical radiometric forces being an estimate of the accommodation coefficient in the Maxwell model. Such a ratio for different gases is presented in Fig. 6. The accommodation coefficients for the Maxwell model, obtained in this work, are 0.81 for argon, 0.86 for xenon, and 0.53 for helium, all of them on a machined aluminum surface. Note that the value of the accommodation coefficient increases with molecular mass, which is consistent with the experimental observation of [38], but contradicts to a hypothesis of Ref. [37].

Comparison of the above accommodation coefficients with those measured in the past is complicated by several factors in addition to their obvious dependence on particular gas and surface material. First, the coefficients obtained in this work are integral, and not incident angle dependent. Therefore, it is difficult to compare them with molecular beam experiments. Second, the coefficients are generally sensitive to the wall and the surrounding gas temperature, and the results should be analyzed for the same temperature regime. Finally, the purity of the surface is very important, as the surface coverage and surface contamination change the accommodation coefficients. The last factor is related to the surface temperature and accociated gas desorption, the surface roughness and multiple gas-surface encounters, and the gas pressure.

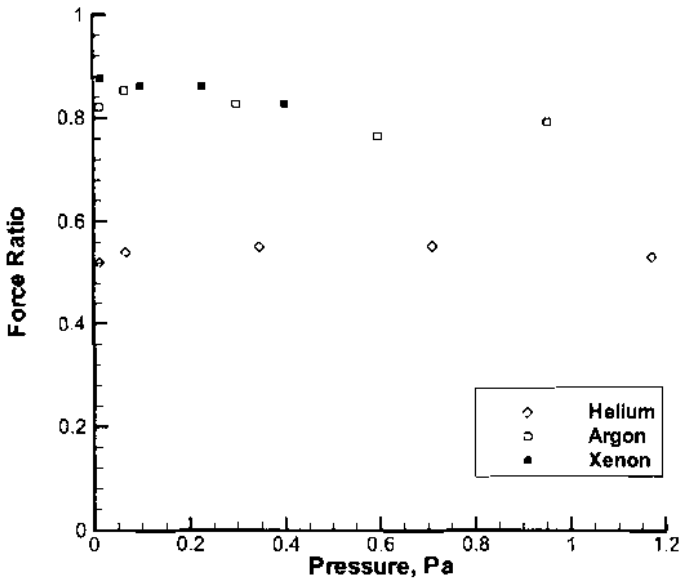

FIG. 6: Experimental-to-computed radiometric force ratio.

For helium, the present accommodation coefficients, 0.53 for the Maxwell model and 0.5 for the Knudsen model, are close to that obtained in Ref. [17] for the thermal accommodation coefficient on machined alumined kept at room temperature, for which the value of 0.47 was measured. The accommodation coefficient of helium on a plasma treated surface obtained in Ref. [17] is lower, 0.38. The normal momentum coefficients recommended [38] for helium on aluminum are somewhat higher, 0.65. It was also shown in Ref. [38] that the efficiency of the momentum transfer process increases with the mass of gas molecules, and relatively weakly depends on the surface material for temperatures ranging from 25°C to 550°C. The tangential momentum coefficients of helium on aluminum are not available, but for other materials were found to vary in a wide range depending on the experimental technique used, from 0.2 [39] to about 0.9 [40].

The thermal accommodation coefficient of argon on aluminum, tabulated in Ref. [16], ranges from 0.334 to 0.75 for different experimental techniques and surface temperatures from 400 K to 800 K. A larger value of 0.86 was measured [17] for argon atoms colliding with a machined aluminum surface. A tangential momentum accommodation coefficient of 0.893 was recommended in Ref. [18] based on the analysis of a large array of experimental

data.

The accommodation of xenon on aluminum has not been extensively studied in the past. The thermal accommodation coefficient was reported for temperatures from 500 K to 800 K as 0.4 Ref. [16], where a concentric-cylinders method was used. Among other materials, platinum was studied theoretically [41], and the energy and momentum accommodation coefficients were calculated for room temperature conditions to be 0.85 and 0.81, respectively. A mean value of 0.95 was recommended in [18] for the tangential momentum accommodation coefficient of xenon on commonly employed surface materials. In measurement [37], this coefficient was estimated as 0.9 for xenon on bronze ribbon.

CONCLUSIONS

A technique for estimation of gas-surface accommodation coefficients, based on the experimental and numerical modeling of radiometric forces on heated vanes in rarefied flows, is presented. The approach applies a new combined ES-BGK kinetic approach to match accurately measured force on a circular radiometer installed on a nano-Newton thrust stand and mounted in a large vacuum chamber. Accommodation coefficients for the Maxwell model of gas-surface interaction may be deduced for a given pressure and gas-surface pair whether through the successive use of the combined approach with different values of the accommodation coefficient, or assuming a linear dependence of radiometric force on the accommodation coefficient.

The combined kinetic approach includes two steps. The first step is the solution of the ES-BGK model equation obtained in the entire chamber. The second step uses the DSMC method applied in a much smaller domain, with the subsonic boundary conditions extracted from the ES-BGK macroparameters based on the incoming molecules. Helium, argon, and xenon were considered in this work, for pressures ranging from approximately 0.01 to 1 Pa, and an aluminum vane with a diameter of 0.113 m was examined. The suggested values of the Maxwell model accommodation coefficients are 0.81 for argon, 0.86 for xenon, and 0.53 for helium, which reasonably agree with momentum and energy accommodation coefficients proposed in the literature. The proposed experimental - computational techniques is general enough to be applied to a wide range of gases, surfaces, and temperature conditions.

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